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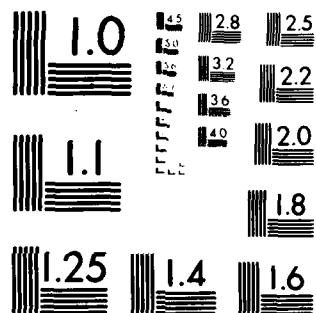
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Volume I

② LEVEL II

**R2D2 — A FORTRAN PROGRAM FOR
TWO-DIMENSIONAL CHEMICALLY REACTING,
HYPERHERMAL, INTERNAL FLOWS**

Volume I — Method of Analysis

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JANUARY 1980

TECHNICAL REPORT AFFDL-TR-79-3162, Volume I
Final Report for period May 1978 — September 1979

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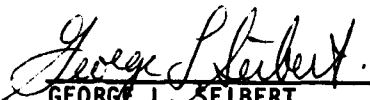
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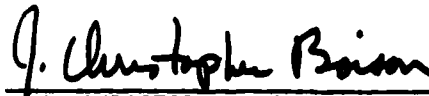
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ities in wall slope are admissible. The axisymmetric formulation includes a swirl component of velocity, in addition to the axial and radial components, which may be significant in swirl-stabilized arc facilities. The current version of R2D2 incorporates a thermochemical data package for an 8 species, 10 chemical reaction model of high temperature air, including ionization and vibrational excitation. However, the number of species and reactions is only limited by considerations of computer storage and running time, which can be formidable.

The system of differential equations is stated for an unsteady flow, and solved in finite difference form subject to steady boundary conditions to determine the asymptotic steady state. An explicit finite difference algorithm is used, placing stringent limitations on the permissible time step, dictated by a combination of wave speed and reaction speed. The initial conditions may consist of either a quasi-one-dimensional frozen flow solution, generated internally by the program, or a stored two-dimensional solution generated previously by the program (subject to the same or different boundary conditions).

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FOREWORD

The work reported herein was conducted by General Applied Science Laboratories, Inc., principally under contract F33615-78-C-3016 issued by the U.S. Air Force, Air Force Systems Command, Air Force Wright Aeronautical Laboratories, Air Force Flight Dynamics Laboratory, Wright-Patterson AFB, Ohio 45433, under the technical Direction of Dr. George Seibert, AFAL/FIME. The work was also partially supported by GASL internal funds.

The report consists of two parts. The first volume describes the theoretical formulation and method of analysis employed in the subject computer program. The second volume is a guide to the use of the program.

The cooperation of Dr. John Lordi of CALSPAN Corp. in furnishing a listing of their one-dimensional, nonequilibrium streamtube program and related reports is gratefully acknowledged. Portions of the CALSPAN code have been incorporated as subroutines of the subject program, thereby providing a degree of commonality with other nonequilibrium flow programs in current use in the Thermomechanics Branch of the Air Force Flight Dynamics Laboratory.

The work was performed during the period 15 May 1978 to 30 September 1979.

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LIST OF SYMBOLS

a	speed of sound
A,B,C,D	components of the Jacobian of the transformational from (x_1, x_2) to (ξ, η) coordinate systems; i.e: $A = \partial \eta / \partial x_1$, $B = \partial \xi / \partial x_1$, $C = \partial \eta / \partial x_2$, $D = \partial \xi / \partial x_2$.
c	number of elements in the mixture of species
C_p	mixture specific heat at constant pressure per unit mass
C_{p_i}	specific heat at constant pressure of i^{th} species, per unit volume
C_v	mixture specific heat at constant volume per unit mass
C_{v_i}	specific heat at constant volume of i^{th} species, per unit volume
e	internal energy per unit mass
E	total internal energy per unit mass; $E = e + \frac{1}{2}(u_1^2 + u_2^2 + u_3^2)$
e_{v_i}	vibrational energy per unit volume of i^{th} species
\dot{e}_{v_i}	time rate of relaxation of vibration energy per unit volume of i^{th} species
e,f,g,h	arrays of dependent variables, defined by Equations (67)-(70)
f	an arbitrary dependent variable, in Equations (63)-(65)
f,g	indices defining the subscript range for species which may be in vibrational nonequilibrium; i.e., $f < i \leq g$. Note: $f < g \leq$ is required
h	mixture enthalpy per unit mass
h_i	enthalpy of i^{th} species, per unit volume
H	total enthalpy per unit mass, $H = h + \frac{1}{2}(u_1^2 + u_2^2 + u_3^2)$
l	total number of chemical species in the mixture. $l \geq c$ is required
L	reference length
MW_i	molecular weight of i^{th} species
\overline{MW}	molecular weight of mixture of species; $\overline{MW} = \sum \gamma_i$
n	distance normal to a surface
p	pressure

LIST OF SYMBOLS (Continued)

Q_{ij}	volumetric rate of production of j^{th} species due to i^{th} chemical reaction
R_0	universal gas constant
r	radial coordinate in a cylindrical system
s	curvilinear distance along a surface
S	entropy per unit mass
t	time
T	temperature
u_1, u_2, u_3	velocity components in the x_1, x_2, x_3 direction
u_{12}	magnitude of the velocity vector in the x_1, x_2 plane; $\sqrt{u_1^2 + u_2^2}$
v_x, v_y	velocity components in a Cartesian (x, y) system
v_r, v_θ, v_z	velocity components in a cylindrical (r, θ, z) system
v_s, v_n	velocity components in a streamline (s, n) system
\dot{w}_i	mass rate of production of i^{th} species by chemical reaction
x_1, x_2, x_3	arbitrary orthogonal coordinates
x, y	Cartesian coordinates
z	axial coordinates in a cylindrical system
γ	ratio of specific heats ($\gamma = \gamma_f$), or the isentropic exponent ($\gamma = \gamma_e$)
γ_i	molar concentration per unit mass of i^{th} chemical species (mass fraction divided by molecular weight)
δ_{ij}	number of atoms of i^{th} element in the j^{th} chemical species
η	azimuthal component of vorticity. Also transformed normal coordinate.
Δ	incremental quantity
θ	azimuthal coordinate in a cylindrical system
θ_{vi}	characteristic vibrational temperature of the i^{th} species
ξ	radial component of vorticity. Also transformed streamwise coordinate

LIST OF SYMBOLS (Continued)

ρ	density
ϕ	angle between s and x_1 coordinates
$\vec{\omega}$	vorticity vector

SECTION I

INTRODUCTION

A hypervelocity arc tunnel can be described¹ as a convergent-divergent duct characterized by (a) a relatively short plenum chamber into which high enthalpy, high pressure gases are introduced from an arc-heater section (possibly mixed with a secondary gas flow) at subsonic velocity, and typically at or near thermochemical equilibrium (but with, perhaps, vibrational excitation), (b) an area contraction into the throat region, and (c) a nozzle section through which the flow expands to supersonic or hypersonic velocity, with concomitant reductions in pressure and temperature, at times (depending on geometry) producing a rapid slowing and/or freeze-out of the chemical reactions and vibrational relaxation in the nozzle section². Due to the relatively short length of the plenum section, the nature of the arc heating process, and the possibly incomplete mixing of primary and secondary gas streams, significant inhomogeneities may exist in the gas flow entering the throat region, both in terms of gas composition, velocity and thermodynamic state. These inhomogeneities will convect through the nozzle, producing uncertainties and possibly spurious effects in the interpretation of test results. The requirement for the computer program which has been developed arises from the need to better understand how these inhomogeneities convect through the tunnel, and to quantitatively assess their effects on the uniformity of the flow produced at the nozzle exit (or test section).

Thus, the flow problem to be numerically solved consists of a nonuniform two-dimensional or axisymmetric high enthalpy flow which may be in or near equilibrium in a plenum, and expands through an arbitrary duct. For the program to be useful for enthalpies up to 10^4 BTU/lbm and pressures to 200 atmospheres, a vibrational energy equation must be included in the system of equations for each diatomic or polyatomic species, as their vibrational states may be characterized by temperatures significantly different than the static temperature. In the axisymmetric case, a swirling flow is often used to stabilize the arc, resulting in an appreciable level of angular momentum in the plenum, which can produce relatively large values of angular velocity at the throat (e.g., in a hypersonic nozzle where $r \rightarrow 0$ at the throat on all streamlines). Thus a

fully justified approach to the axisymmetric problem must also include the angular momentum equation in the system. Currently available one-dimensional analyses^{2,3} cannot account for either swirl or radial nonuniformities of inlet flow properties, and two-dimensional analyses appear to be limited to supersonic reacting flows⁴ or perfect gases^{5,6}.

In response to these requirements, General Applied Science Laboratories, Inc., has developed Program R2D2, a Fortran code for two-dimensional chemically reacting, vibrationally excited, hyperthermal, inviscid flow in a duct, which includes swirling axisymmetric flow. The program name R2D2 refers to its evolution from two pre-existing codes; one for one-dimensional steady reacting flows and the other for two-dimensional, unsteady swirling duct flows. Two versions of the program have been produced. The first, R2D2NE, is for general nonequilibrium flows, which may include equilibrated vibration as well as nonequilibrium vibrational excitation. The second, R2D2EQ, is for fully equilibrated flows.

SECTION 2

GENERAL OUTLINE OF THE APPROACH

1. TIME-DEPENDENT METHOD

The technique of determining the steady state solution of a mixed flow (subsonic, transonic and supersonic regions) as the asymptote of an unsteady process is now well established. The present approach can be considered an extension of the one-dimensional, chemically reacting flow analysis of Anderson³, for example, to two-dimensional flows. The widely used explicit, second-order accurate, finite difference algorithm developed by McCormack⁷, also used by Anderson³, has been adopted in view of its simplicity and reliability. Although more efficient implicit algorithms are gaining popularity, their application to large systems of coupled equations, as are encountered in multicomponent reacting gases, is still the subject of current research.

The selection and application of inlet and exit boundary conditions for internal flows warrants careful exposition, particularly where the flow is choked by a throat in the duct. Consideration of a chemically reacting flow places an additional constraint on the proper boundary conditions. the selected boundary conditions should, of course, yield a unique as well as steady solution. Thus, they must allow the influence of initial conditions to decay with the passage of time, such that the asymptote is indeed independent of the initial conditions. Finally, the selected finite difference grid should conform to the duct wall contours, along which the sole boundary condition of impermeability is to be enforced. In addition, it should afford a degree of flexibility in matching the grid spacing to the geometric variations of the duct. The present approach to meeting these general requirements of the time-dependent method are outlined as follows.

2. BOUNDARY CONDITIONS

It will be seen in the following section that casting the system of equations in characteristic form, at least approximately, provides useful guidelines for determining the number and type of boundary conditions to be imposed at the boundary surfaces of the computational domain. The characteristic form is also often useful in implementing a second-order accurate solution algorithm at the boundary points.

The wall surface boundary condition is well known; impermeability requires a vanishing component of velocity normal to the surface. the normal component

of velocity must also vanish at an axis of symmetry. However, the inlet and exit boundary conditions are not so easily dismissed. It can be shown^{5,8} that at a subsonic inflow boundary (i.e., flow crossing into the computational domain) all flow properties except one must be specified a priori, and at a supersonic inflow boundary all must be specified. In the former case, one property must be allowed to change in time in accord with the requirements of the upstream travelling waves crossing the boundary. In a choked flow, the waves reflected off the throat must be allowed to change the inlet mass flow rate until a steady state is reached. In an unchoked subsonic flow the waves reflected off the exit boundary perform the same function. However the thermochemical state of the inlet flow must also be specified as a boundary condition. Therefore, the thermodynamic properties at the inlet, e.g., the density or temperature cannot be allowed to change in time. Consequently, the axial velocity must be selected as the inlet flow property to be determined by the outgoing waves.

It is also easily shown^{5,8} that at a supersonic outflow boundary (i.e., the flow crossing out of the computational domain) no boundary condition can be imposed, and at a subsonic outflow boundary, only one boundary condition can be imposed. In the latter case, the static pressure is the usual choice.

In an unchoked subsonic duct flow, this combination of boundary conditions does not yield a unique solution, since a variety of mass flow rates (i.e., axial velocities) can satisfy the stated conditions. (This is not an unusual inviscid flow situation.) In this case one can expect, at best, the solution closest to the initial conditions. However, in a choked flow, the mass flow is fixed by the throat size, and uniqueness follows. In a supersonic flow, uniqueness is again guaranteed, even if the flow recompresses to subsonic speed at the exit (e.g., the back pressure will control the normal shock position).

3. INITIAL CONDITIONS

The solution may be initialized in one of two ways. If no other information is available, a quasi-one-dimensional solution can be generated by Program R2D2 assuming uniform total pressure, total temperature and Mach number at each station in the duct and iterating the Mach number until a specified initial mass flow rate is matched. (There is no guarantee that it can be matched to within an arbitrary tolerance in the vicinity of a throat. In this case the specified initial mass flow rate must also be iterated to match the choking mass rate as closely as

desired.) The resulting velocity vectors are then rotated to satisfy the wall and/or axis boundary conditions, and their directions linearly interpolated between these boundaries. The iteration procedure assumes a dropping pressure in the downstream direction to start the iteration at each station. Thus it usually converges on the supersonic branch downstream of a throat; however, the desired branch cannot be guaranteed since both subsonic and supersonic solutions can satisfy the mass flow criterion. In some cases, a small change in the specified initial mass flow rate can change the branch on which the procedure converges. In addition, it must be recognized that this procedure ignores the boundary conditions to be imposed at the inlet and exit stations. Thus the boundary conditions are, in fact, imposed impulsively on the first time step. The magnitude of the impulse should be minimized by consistent determination of initial mass flow rate, total pressure and total temperature.

The initialization procedure for an axisymmetric flow includes conservation of angular momentum, based on inlet boundary conditions, along streamwise grid rows, which are reasonably good approximations to streamlines. In the non-equilibrium version of the program, the species concentrations and vibrational temperatures are initialized by conserving their inlet boundary values along streamwise grid rows. The validity of the assumption of a frozen flow as the initial state is highly dependent on the particular duct geometry and inlet pressure and temperature. A rapid transient in the thermochemical state frequently ensues due to this aspect of the initialization, which could be remedied (in the future) by provision for an equilibrium option in the initialization.

The equilibrium version of the program initializes to a complete equilibrium state, based on the initial temperature and pressure field.

The second procedure available for initializing the solution is to use a previously stored solution, which utilized the same grid dimensions and either the same or different boundary conditions and/or duct geometry. This procedure is intended primarily to permit restarting a solution which has not completely converged on a steady state. However, it may be utilized to good advantage in a parametric study, for example, by initializing each solution to a known baseline solution, or to the preceding solution in a systematic variation of parameters.

4. GRID GENERATION

The efficiency and accuracy of the finite difference solution is clearly dependent upon selection of an appropriate (and adequate) grid system. Program R2D2 has adopted the basic grid generation scheme of the duct flow program from which it derives⁸, in large part because it admits discontinuities in wall slope. It does, however, produce a non-orthogonal grid which is limited to uniformly spaced radial and axial intervals between the boundaries of each computational domain (i.e., an upper wall, a lower wall or axis, an inlet station and an exit station). Since it is non-orthogonal, the elements of the Jacobian of the transformation are calculated and stored at each grid point. Consequently, the grid generation subroutine could easily be replaced by any other non-orthogonal (or orthogonal) grid generation procedure which meets the general requirement of equal spacing in a transformed coordinate system and duct boundaries mapped to the boundaries of the grid system.

The first step in the present grid generation procedure is to divide the complete computational volume into a sequence of contiguous domains, within which the number of grid volumes and rows can be independently specified. Furthermore, the wall slopes need be continuous within a domain, but may be discontinuous at the interface between domains. The general arrangement of a sequence of domains is sketched in Figure (1).

The number of grid columns in each domain is arbitrary subject to the limitation that the sum of the number of domains and the total number of grid columns in all domains is less than an upper bound:

$$I_{\text{dom}} + \sum_{j=1}^{I_{\text{dom}}} J_{\text{max}j} \leq J_{\text{bound}} \quad (1)$$

where J_{bound} is 50 in the current version of R2D2.

The number of grid rows in each domain is also arbitrary, subject to the limit:

$$K_{\text{max}j} \leq K_{\text{bound}} \quad (2)$$

where K_{bound} is 21 in the current version of R2D2.

The physical Cartesian or cylindrical coordinates, (x,y) or (z,r) , are transformed in an (ξ,η) system in each domain by defining

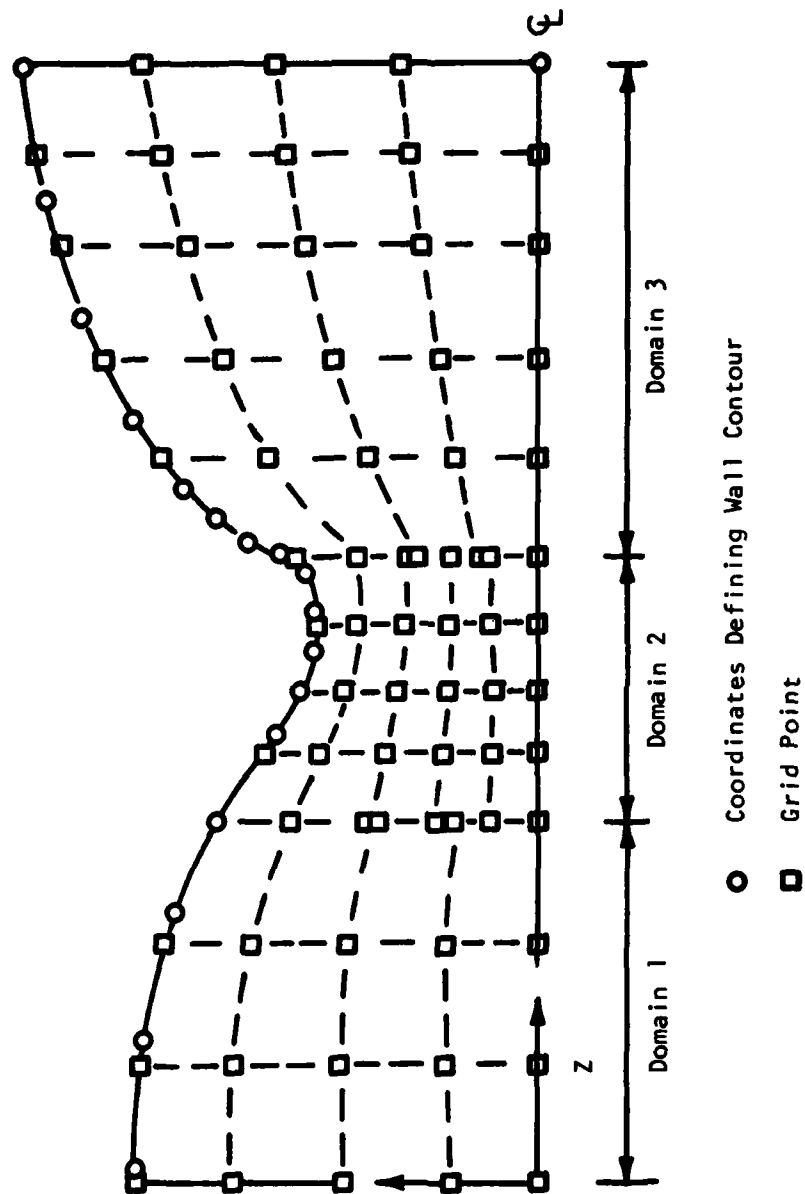


FIGURE 1. SCHEMATIC OF A CONVERGING-DIVERGING DUCT, SHOWING THREE COMPUTATIONAL DOMAINS, WITH A 4×5 GRID IN THE FIRST, A 5×6 IN THE SECOND, AND A 6×5 IN THE THIRD, AND A DISCONTINUITY IN WALL SLOPE BETWEEN THE SECOND AND THIRD DOMAINS.

$$\xi_i = \left[\frac{x - x_R}{x_L - x_R} \right]_i \quad \text{or} \quad \left[\frac{z - z_R}{z_L - z_R} \right]_i \quad (3)$$

$$\eta_i = \left[\frac{y - y_H}{y_T - y_H} \right]_i \quad \text{or} \quad \left[\frac{r - r_H}{r_T - r_H} \right]_i \quad (4)$$

$$\text{where} \quad x_L = x_L(y) \quad \text{or} \quad z_L = z_L(r) \quad (5a)$$

$$x_R = x_R(y) \quad \text{or} \quad z_R = z_R(r) \quad (5b)$$

$$y_H = y_H(x) \quad \text{or} \quad r_H = r_H(z) \quad (5c)$$

$$y_T = y_T(x) \quad \text{or} \quad r_T = r_T(z) \quad (5d)$$

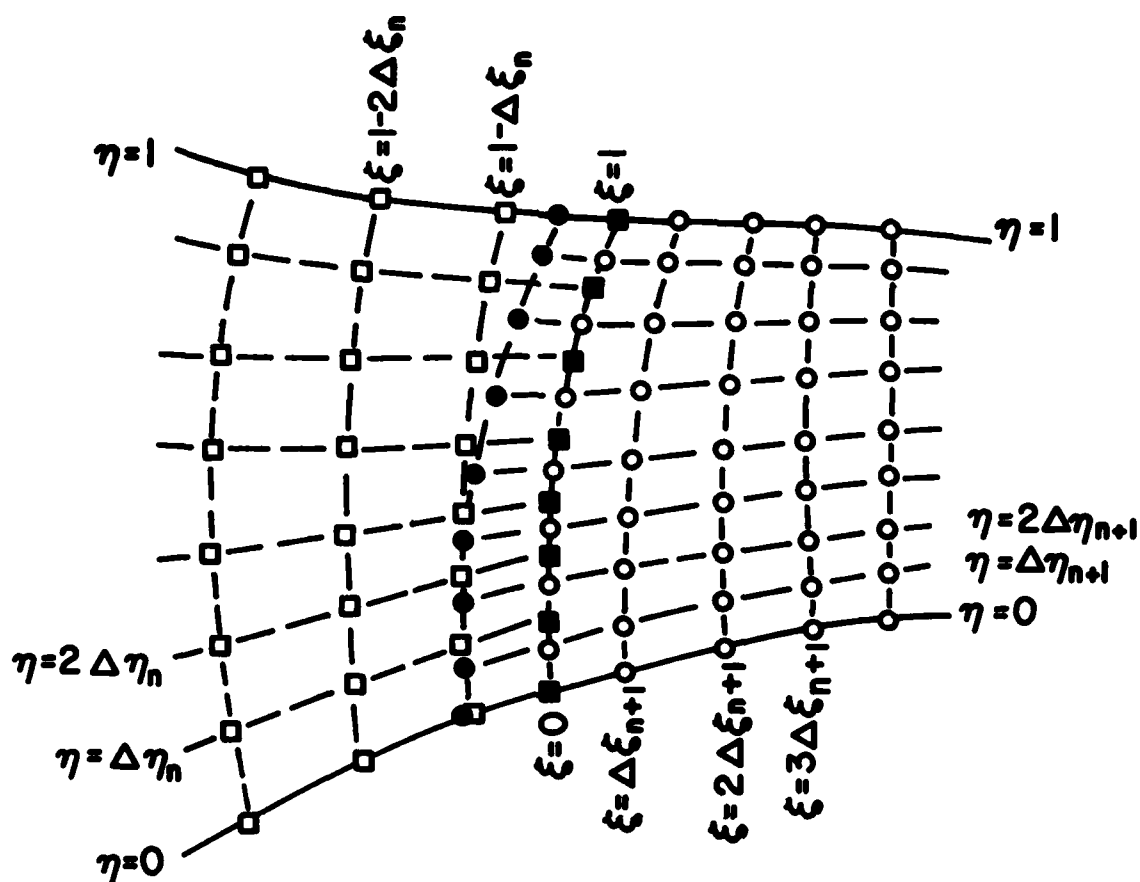
are the coordinates of the left and right side (inlet and exit) boundaries of the i^{th} domain and of the hub (axis) or lower wall and top (upper) wall of the duct. The left and right boundaries are assumed to be straight but not necessarily vertical. The lower and upper walls of the duct are specified by a series of arbitrarily spaced coordinates, which are fit by a cubic spline curve⁹ within each domain.

A rectangular grid in the transformed (ξ, η) system is defined by:

$$\Delta \xi_i = 1/(J_{\max i} - 1) \quad (6a)$$

$$\Delta \eta_i = 1/(K_{\max i} - 1) \quad (6b)$$

Obviously, the last grid line of the i^{th} domain, $\xi_i = 1$, is, by definition, coincident with the first line of the next domain $\xi_{i+1} = 0$. Patching of solutions along the interface between domains is accomplished by defining a vertical grid column at $\xi_i = -\Delta \xi_i$ for every domain (except the first), which therefore overlaps into the preceding domain, as shown in Figure (2). Grid columns at $\xi_i = 0, \Delta \xi_i, 2\Delta \xi_i, \dots, 1-\Delta \xi_i$ are considered "interior columns", while the columns at $\xi_i = -\Delta \xi_i$ and $\xi_i = 1$ are considered "virtual columns". The solution at the "interior columns" is advanced by the finite difference algorithm,



- INTERNAL GRID POINT OF n^{TH} DOMAIN
- EXTERNAL GRID POINT OF n^{TH} DOMAIN
- INTERNAL GRID POINT OF $(n+1)^{\text{TH}}$ DOMAIN
- EXTERNAL GRID POINT OF $(n+1)^{\text{TH}}$ DOMAIN

FIGURE 2. GRID POINT ARRANGEMENT AT INTERFACE BETWEEN n^{TH} AND $(n+1)^{\text{TH}}$ DOMAINS

while the solution at the "virtual columns" is interpolated from the "interior columns".

Note, first of all, that the complete computational volume is covered by "interior columns" of grid points; the virtual columns are artifices introduced for convenience in patching the domains together. Second, a one-dimensional linear interpolation is required at points along $\xi_i = 1$ if $K_{\max i} \neq K_{\max i+1}$, whereas a two-dimensional linear interpolation is required at points along $\xi_i = -\Delta\xi_i$ if $(x_L - x_R)_i / (J_{\max i} - 1) \neq (x_L - x_R)_{i+1} / (J_{\max i+1} - 1)$ and $K_{\max i} \neq K_{\max i+1}$. Third, the choices of values of $J_{\max i}$, $K_{\max i}$, l_{dom} and of domain boundaries are almost entirely arbitrary. This degree of flexibility is intended to allow the user to tailor the grid system such that adequate resolution can be obtained where it is needed without burdening other areas with excessive numbers of grid points, as well as to accommodate discontinuities in wall slope. However, the user should be cautioned that, as a rule of thumb, large changes in grid size across a domain interface, and ratios of grid sizes in the two directions substantially different than unity, are to be avoided. Abrupt changes in grid size across a domain interface tend to interfere with proper propagation of waves across the interface by filtering out and/or reflecting the short wave length components, which cannot be resolved by the larger grid size. Large differences in the grid sizes in the two directions tends to accentuate the numerical diffusion in the direction of the larger grid size, since the smaller grid size will control the time step. In cases where large ratios of grid size are dictated by physical considerations, e.g., within a boundary layer, grid-splitting techniques can be applied to the basic McCormack algorithm to improve its accuracy and efficiency⁷. However, grid splitting has not been incorporated into the current version of program R2D2.

SECTION 3

DESCRIPTION OF THEORY

1. GOVERNING EQUATIONS

The system of partial differential equations describing the continuum fluid mechanics of a mixture of chemically reacting and/or vibrationally relaxing gases is, of course, well established, cf. References (10) and (11). Analytical solutions are limited to highly idealized situations, and recourse to numerical solutions is generally required for practical problems. In the present program, the system of equations is to be solved by finite difference techniques. Consequently, very little derivation is involved in proceeding from the familiar form in which the system is usually stated to the final form in which the differentials are replaced by differences.

The present program was constructed utilizing portions of a GASL program written for two-dimensional internal flow of a perfect gas⁸ and portions of a CALSPAN program written for one-dimensional chemically reacting-vibrationally relaxing flow^{12,13,14}. Therefore, it was necessary to first adopt a consistent system of nondimensionalization that would be applicable to both programs. Thereafter, development of the two-dimensional reacting duct flow program R2D2, was largely a matter of logic and proper interfacing of the components. Description of the governing equations is thus arranged in corresponding fashion.

a. EQUATIONS OF STATE AND NONDIMENSIONALIZATION

The governing system of equations can be completely nondimensionalized by choosing two thermodynamic properties, a length, L , a molecular weight, MW_∞ , and the universal gas constant, R_O , as the scale factors. The choice of thermodynamic properties is arbitrary, but reduction of the equation of state, which must be used repeatedly in the program, to a convenient form provides one rationale. We have selected the pressure, P_∞ , and temperature, T_∞ , as the two basic thermodynamic properties.

A reference density can then be obtained from the equation of state;

$$\rho_\infty = p_\infty MW_\infty / (R_O T_\infty) \quad (7)$$

and a reference velocity can be defined by

$$a_{\infty} = (R_0 T_{\infty} / MW_{\infty})^{\frac{1}{2}} = (p_{\infty} / \rho_{\infty})^{\frac{1}{2}} \quad (8)$$

Obviously, this reference velocity differs from a true speed of sound by a factor of the square root of the isentropic exponent, γ .

The resulting system of scale factors by which variables are nondimensionalized is summarized in Table I. In particular, note that the nondimensional equation of state is:

$$p = \rho T / MW = \rho T \sum \gamma_i \quad (9)$$

and the nondimensional sound speed is:

$$a = (\gamma p / \rho)^{\frac{1}{2}} \quad (10)$$

where γ is the appropriately defined isentropic exponent.

b. FLUID MECHANICS

The conservation laws for mass, momentum and energy for a two-dimensional flow are:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_1}{\partial x_1} + \frac{\partial \rho u_2}{\partial x_2} + j \frac{\rho u_2}{x_2} = 0 \quad (11)$$

$$\frac{\partial \rho u_1}{\partial t} + \frac{\partial (\rho u_1^2 + p)}{\partial x_1} + \frac{\partial \rho u_1 u_2}{\partial x_2} + j \frac{\rho u_1 u_2}{x_2} = 0 \quad (12)$$

$$\frac{\partial \rho u_2}{\partial t} + \frac{\partial \rho u_1 u_2}{\partial x_1} + \frac{\partial (\rho u_2^2 + p)}{\partial x_2} + j \frac{p}{x_2} (u_2^2 - u_1^2) = 0 \quad (13)$$

TABLE I
SCALE FACTORS FOR NONDIMENSIONALIZATION

VARIABLE	SCALE FACTORS		
	Present	Reference (8)	References (12)-(14)
t, time	L/a_∞	L/a_∞	None
p, pressure	p_∞	$p_\infty a_\infty$	p_∞
ρ , density	ρ_∞	ρ_∞	ρ_∞
T, temperature	T_∞	$a_\infty^2 MW_\infty / R_O$	T_∞
v, velocity	a_∞	a_∞	a_∞
H, h, mixture enthalpy and E & e, internal energy*	a_∞^2	a_∞^2	$MW_\infty / R_O T_\infty$
h_i & e_i , species enthalpy and internal energy*	$R_O T_\infty$	None	$R_O T_\infty$
C_p, C_v , mixture specific heat	MW_∞ / R_O	None	MW_∞ / R_O
C_{p_i}, C_{v_i} , species specific heat	R_O	None	R_O
MW, species molecular weight	MW_∞	None	MW_∞
\dot{w}_i , mass rate of production of i th species	$L/\rho_\infty a_\infty$	None	$L/\rho_\infty a_\infty$

*Includes vibrational energy

$$j \left\{ \frac{\partial \rho x_2 u_3}{\partial t} + \frac{\partial \rho x_2 u_1 u_3}{\partial x_1} + \frac{\partial \rho x_2 u_2 u_3}{\partial x_2} + \rho u_2 u_3 \right\} = 0 \quad (14)$$

$$\frac{\partial \rho E}{\partial t} + \frac{\partial \rho u_1 H}{\partial x_1} + \frac{\partial \rho u_2 H}{\partial x_2} + j \frac{\rho u_2 H}{x_2} = 0 \quad (15)$$

where:

$$j = \begin{cases} 0 & \text{for planar flow} \\ 1 & \text{for axisymmetric flow} \end{cases} \quad (16)$$

$$(x_1, x_2) = \begin{cases} (x, y) \\ (z, r) \end{cases} \text{ for } j = \begin{cases} 0 \\ 1 \end{cases} \quad (17)$$

$$(u_1, u_2, u_3) = \begin{cases} (v_x, v_y, 0) \\ (v_z, v_r, v_\theta) \end{cases} \text{ for } j = \begin{cases} 0 \\ 1 \end{cases} \quad (18)$$

$$E = H - p/\rho \quad (19)$$

$$H = h + \frac{1}{2} (u_1^2 + u_2^2 + u_3^2) \quad (20)$$

This system, as stated, is not complete without some constitutive relationship providing $h=h(p,\rho)$. Toward this end, the thermodynamic definition of static enthalpy is introduced:

$$h = \sum_i \alpha_i h_i / MW_1 = \sum_i \gamma_i \left(\int_0^T c_{p_i} dT + \Delta h_i^0 + e_{v_i}(T_{v_i}) \right) \quad (21)$$

where

$$c_{p_i} = c_{p_i}(T) \quad (22)$$

$$\gamma_i = \gamma_i(\rho, T, t, \gamma_j) \quad (23)$$

$$T_{v_i} = T_{v_i}(\rho, T, t, \gamma_j) \quad (24)$$

The dependence of γ_i and T_{v_i} on time and on the other chemical constituents relates to nonequilibrium flows, in which solution of the species conservation equation is required to determine γ_i , and solution of the vibrational energy equation provides the vibrational temperature, T_{v_i} . The dependence of T_{v_i} on γ_j is introduced by vibration-dissociation coupling models^{12,14}. In an equilibrium flow $\gamma_i = \gamma_i(\rho, T)$ and $T_{v_i} = T$, but the functional relationship is usually very complex and therefore expressed graphically, rather than analytically. The functional dependence of species specific heat on temperature is also typically non-analytical, except for very simple molecules. Consequently, Equations (11), (15) and (19)-(21) seldom yield an analytical solution for temperature. Therefore, an analytical relationship of the form $h = h(p, \rho)$ is generally unattainable (in either nonequilibrium or equilibrium flows) except for idealized systems. The usual procedure is to determine $T = T(h, \gamma_i)$ by iterative solution of Equation (21). Since the iteration would have to be carried out at every grid point on each time step, it could represent a substantial computational burden in the present program. Therefore, it is considered highly advantageous to rewrite the energy equation in terms of the temperature rather than enthalpy or internal energy, to avoid this iteration. Derivation of the temperature form of the energy equation may proceed from the second law of thermodynamics:

$$\frac{De}{Dt} + p \frac{D}{Dt} \left(\frac{1}{\rho} \right) = 0 \quad (25)$$

$$\text{where } e = h - p/\rho \quad (26)$$

$$\text{and } D/Dt = \partial/\partial t + u_1 \partial/\partial x_1 + u_2 \partial/\partial x_2 \quad (27)$$

Utilizing the equation of state and the definition of static enthalpy, this equation becomes:

$$C_v \frac{DT}{Dt} = \frac{p}{\rho^2} \frac{D\rho}{Dt} - \sum \gamma_i \frac{De_{vi}}{Dt} - \sum e_i \frac{D\gamma_i}{Dt} \quad (28)$$

This may now be combined with the Continuity Equation to yield:

$$\begin{aligned} \frac{\partial \rho T}{\partial t} + \frac{\partial \rho u_1 T}{\partial x_1} + \frac{\partial \rho u_2 T}{\partial x_2} = & -(\gamma_f - 1) \rho T \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} \right) \\ & - j \gamma_f \rho T \frac{u_2}{x_2} - \frac{p}{C_v} \left(\sum \gamma_i \frac{De_{vi}}{Dt} + \sum e_i \frac{D\gamma_i}{Dt} \right) \end{aligned} \quad (29)$$

$$\text{where } e_i = h_i - R_o T \quad (30)$$

$$C_p = \sum \gamma_i C_{pi} \quad (31)$$

$$C_v = C_p - R_o \sum \gamma_i = \sum \gamma_i C_{vi} \quad (32)$$

$$\text{and } \gamma_f = C_p / C_v \quad (33)$$

This form of the equation is applicable to nonequilibrium flows, wherein the terms involving the LaGrangian derivatives of the vibrational energy and species concentration can be replaced by rate expressions. In an equilibrium flow the corresponding equation can be obtained by introducing an isentropic exponent defined by

$$\gamma_e = \left(\frac{\partial \ln p}{\partial \ln \rho} \right)_{S=\text{constant}} \quad (34)$$

$$\text{or } p = k \rho^{\gamma_e} \exp(S) \quad (35)$$

where the entropy, S , satisfies Equation (25) if:

$$\frac{DS}{Dt} = 0 \quad (36)$$

It then follows that

$$\begin{aligned} \frac{\partial \rho T}{\partial t} + \frac{\partial \rho u_1 T}{\partial x_1} + \frac{\partial \rho u_2 T}{\partial x_2} = -(\gamma_e - 1) T \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} \right) \\ - j \gamma_e \rho T \frac{u_2}{x_2} + \rho T \frac{D \ln \overline{MW}}{Dt} \end{aligned} \quad (37)$$

Equations (29) and (37) are adopted as the nonequilibrium and equilibrium forms of the Energy Equation, respectively. It should be recognized, however, that Equations (29) and (37) are restricted to shock-free flows, whereas the originally stated form, Equation (15) is not. In addition, with respect to the above equation, it should be pointed out that the mixture molecular weight only changes significantly if the molecular composition of the mixture undergoes rather severe changes, e.g., from primarily diatomic to monatomic molecules. Thus, under a wide range of conditions of practical interest, e.g., air at temperatures up to about 7000°K and pressures above 10⁻² atmospheres, the last term in Equation (37) is negligible.

c. NONEQUILIBRIUM CHEMICAL KINETICS AND VIBRATIONAL RELAXATION

A nonequilibrium flow may be characterized by a time constant for chemical rate processes and/or vibrational relaxation which is of the same order or slower than that for wave propagation. This characterization is subsequently put on a more quantitative basis in the context of stability considerations for the finite difference algorithm. If the flow is out of equilibrium with respect to chemical composition and/or vibrational state, the preceding system of fluid mechanical equations must be supplemented with a system of rate equations describing the conservation of chemical species and vibrational energy. These are written as:

$$\begin{aligned} \frac{\partial \rho \gamma_i}{\partial t} + \frac{\partial \rho u_1 \gamma_i}{\partial x_1} + \frac{\partial \rho u_2 \gamma_i}{\partial x_2} + j \rho u_2 \gamma_i / x_2 = \frac{\dot{w}_i}{MW_i} = \frac{1}{u_{12}} \sum_j Q_{ji} \end{aligned} \quad (38)$$

$i = 1, 2, 3, \dots, I$

$$\frac{\partial \rho e_{vj}}{\partial t} + \frac{\partial \rho u_1 e_{vj}}{\partial x_1} + \frac{\partial \rho u_2 e_{vj}}{\partial x_2} + j \rho u_2 e_{vj} / x_2 = \rho \dot{e}_{vj} \quad (39)$$

$$j = f+1, f+2, f+3, \dots, g$$

where the mixture of gases is composed of I species, of which those in the range $f < i \leq g$ are assumed to be undergoing vibrational relaxation. The vibrational states of the species in this range are characterized by a Boltzmann distribution at a temperature $T_{vj} \neq T$. The vibrational energy is thus expressed in terms of T_{vj} as:

$$e_{vj} = (\theta_{vj}/T_{vj}) / (\exp(\theta_{vj}/T_{vj}) - 1.0) \quad (40)$$

The species in the ranges $1 \leq i \leq f$ and $g < i \leq I$ may also possess vibrational degrees of freedom, but they are assumed to be fully equilibrated, i.e., $T_{vj} = T$.

The mixture of I chemical species may be composed of c elements ($c \geq 1$). Since elements cannot be created or destroyed by the reactions, Equations (38) must contain a subset for which:

$$\frac{\partial \tilde{\gamma}_i}{\partial t} + \frac{\partial \rho u_1 \tilde{\gamma}_i}{\partial x_1} + \frac{\partial \rho u_2 \tilde{\gamma}_i}{\partial x_2} + j \rho u_2 \tilde{\gamma}_i / x_2 = 0 \quad (41)$$

$$i = 1, 2, 3, \dots, c$$

where:

$$\tilde{\gamma}_i = \sum_{j=1}^I \delta_{ij} \gamma_j \quad (42)$$

and the δ_{ij} coefficient matrix is composed of numbers of atoms of elements in species j . It therefore follows that:

$$\sum_{j=1}^I \delta_{ij} \dot{\gamma}_j = 0 = \sum_{j=1}^c \delta_{ij} \dot{\gamma}_j + \sum_{j=c+1}^I \delta_{ij} \dot{\gamma}_j \quad (43)$$

$$i=1, 2, 3, \dots, c$$

$$\text{or } (\dot{w}_i) = |\delta_{cc}|^{-1} |\delta_{cI}| |\dot{w}_j| \quad (44)$$

$$i = 1, 2, 3, \dots, c$$

where $|\delta_{cc}|$ denotes the square matrix composed of the first c columns of the δ_{ij} matrix, $|\delta_{cI}|$ represents the remainder of the δ_{ij} matrix (i.e., columns $c+1$ to I), and $|\dot{w}_j|$ denotes the array \dot{w}_j from $j=c+1$ to I . Thus it is, in fact, only necessary to evaluate the chemical production terms for species $c+1$ through I to determine the values of \dot{w}_i for all species.

Note that Equations (38) and (39) can also be written as

$$\frac{D\gamma_i}{Dt} = \frac{\dot{w}_i}{\rho MW_i} \quad (45)$$

$$\frac{De_{vj}}{Dt} = \dot{e}_{vj} \quad (46)$$

or, for example,

$$\gamma_i(x_1, x_2, t) = \gamma_i(x_1 - \Delta x_1, x_2 - \Delta x_2, t - \Delta t) + \frac{1}{MW_i} \int_t^{t+\Delta t} \frac{\dot{w}_i}{\rho} dt \quad (47)$$

$$\text{where } \frac{\Delta x_1}{u_1} = \frac{\Delta x_2}{u_2} = \Delta t \quad (48)$$

The latter form of the equations is useful along known stream surfaces, such as the walls and axis of symmetry which automatically satisfy the conditions $\Delta x_1/u_1 = \Delta x_2/u_2$.

The chemical production terms are evaluated from the Law of Mass Action and a set of specified reaction rates as applied to a system of chemical reactions in accord with well known procedures. The reader is referred to References (12)-(14) for the specific details of the procedure used in the present program, or Reference (15) and (16) for a general overview.

d. EQUILIBRIUM FLOW

A flow in which the characteristic time constants for all relevant chemical and/or vibrational rate processes are much smaller than that for wave propagation is considered to be in thermochemical equilibrium. This condition is in a sense a singular perturbation of the nonequilibrium formulation since the chemical composition, γ_1 , and vibrational energies, e_{v1} , should not be considered to be functions of (x_1, x_2, t) , but rather of pressure and temperature (p, T) . In an equilibrium flow, the fluid mechanical system of equations uncouples from the thermochemical state except for the constitutive relationship required to define $\gamma_e(p, T)$ and $\overline{MW}(p, T)$. (See Equations (9) and (37)).

2. CHARACTERISTIC FORM OF INLET/OUTLET BOUNDARY CONDITIONS

Assume, for the moment, that the flow within a distance Δx_1 of the inflow, or outflow, surface is either in local equilibrium, or locally frozen. The energy equation then assumes the familiar form given by Equation (36):

$$S = \text{constant} \quad (49a)$$

$$\text{on} \quad \frac{dx_1}{u_1} = \frac{dx_2}{u_2} = dt \quad (49b)$$

which can be combined with the equations of continuity and axial momentum to obtain:

$$\frac{d \log p}{dt} + \frac{\gamma}{a} \frac{du_1}{dt} = \frac{\gamma}{x_2^j} \frac{\partial}{\partial x_2} (x_2^j u_2) \quad (50a)$$

$$\text{on} \quad \frac{dx_1}{u_1 + a} = \frac{dx_2}{u_2} = dt \quad (50b)$$

where γ and a are the equilibrium or frozen isentropic exponent and sound speed, respectively. A planar surface parallel to the (x_1, t) plane and translating in the x_2 direction at a velocity u_2 is referred to as the reference plane in which Equations (49a) and (50a) can be integrated along the lines defined by Equations (49b) and (50b). The reference plane and characteristic

lines are depicted in Figure (3).

It should be noted that the angular momentum equation, the species and elemental conservation equations, and the vibrational energy equation can also be written in the form:

$$j \frac{D}{Dt} (x_2 u_3) = 0 \quad (51)$$

$$\frac{D\tilde{\gamma}_i}{Dt} = 0 \quad (52)$$

$$\frac{D\gamma_i}{Dt} = \dot{w}_i / \rho \quad (53)$$

$$\frac{De_{vi}}{Dt} = e_{vi} \quad (54)$$

on $\frac{dx_1}{u_1} = \frac{dx_2}{u_2} = dt \quad (55)$

Thus, it is clear that the entropy, angular momentum, gas composition and vibrational energy are all convective properties of the flow. This statement may be augmented by noting that the curl of the momentum equation may be combined with the continuity equation to yield the vorticity transport equation:

$$\frac{D}{Dt} \left(\frac{\vec{\omega}}{\rho} \right) = \frac{\vec{\omega}}{\rho} \cdot \nabla \vec{V} \quad (56a)$$

on $\frac{dx_1}{u_1} = \frac{dx_2}{u_2} = dt \quad (56b)$

Therefore, the vorticity (or more precisely the ratio of vorticity to density) is also a convective property of the flow. Consequently, all these properties of the flow or equivalent combinations of flow variables, must be specified as boundary conditions at an inflow station, since their characteristic lines

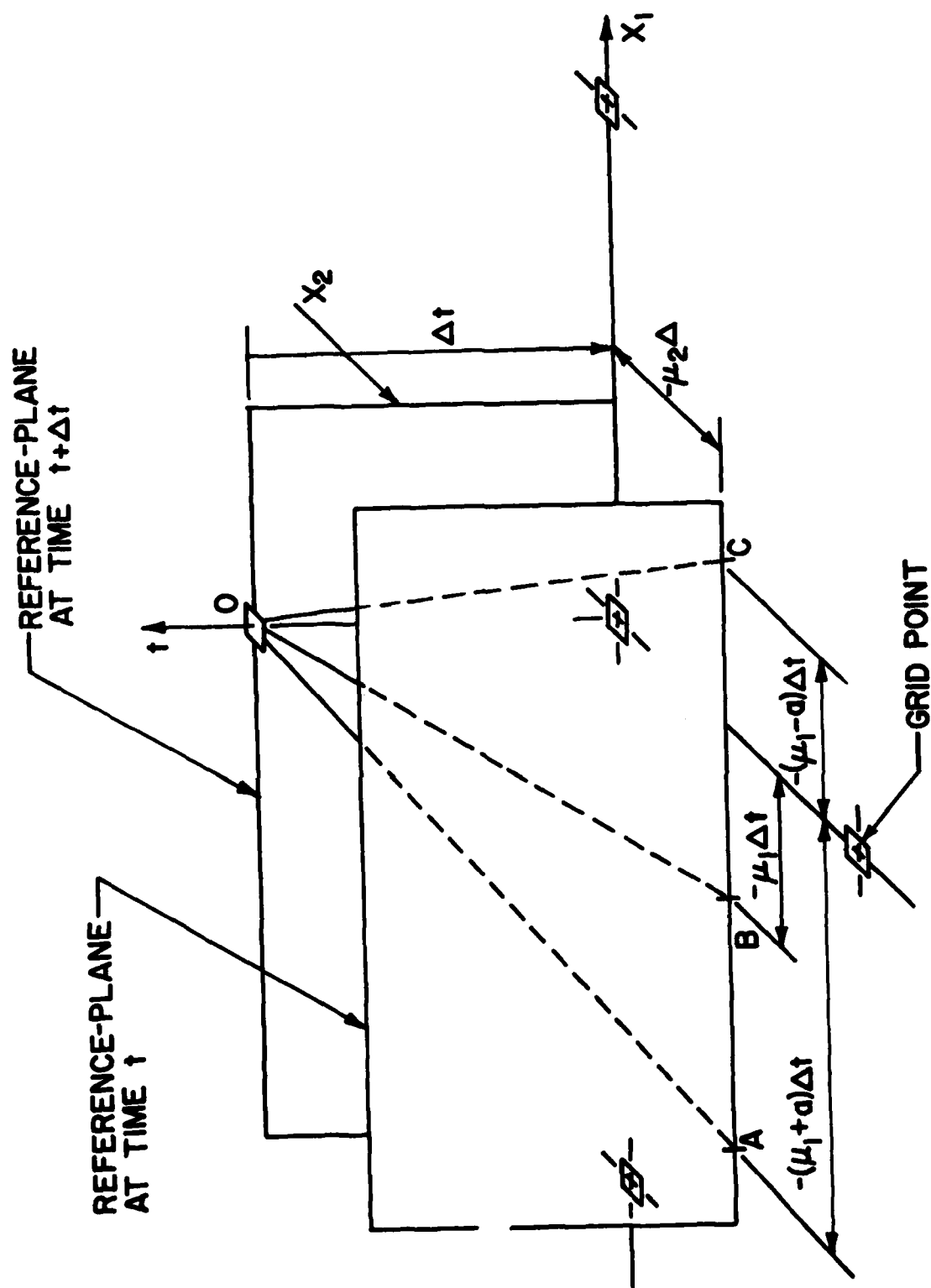


FIGURE 3. REFERENCE-PLANE CHARACTERISTIC SYSTEM
USED AT INLET AND DISCHARGE STATIONS

(which are streampaths) originate upstream of an inflow station (see Figure 3). Conversely, none of these variables may be specified as boundary conditions at an outflow station, since their characteristic lines originate within the computational domain upstream of an outflow station.

The radial momentum and energy equation can be combined to yield

$$\frac{\partial u_2}{\partial t} = T \frac{\partial S}{\partial x_2} - \frac{\partial H}{\partial x_2} + j u_3 \xi - u_1 \eta \quad (57)$$

where ξ and η are components of the vorticity vector $\vec{\omega}$. Therefore, the time rate of change of u_2 at the boundary points along an outflow boundary is determined by the (known) flow properties along the boundary. Thus, Equation (57) can be integrated by the same finite difference algorithm used at the interior points. If the vorticity is specified at an inflow boundary, then Equation (57) may be solved along the inflow boundary points. However, if the vorticity is not specified as a boundary condition, then Equation (57) must be replaced by a specification of u_2 or (u_2/u_1) along the inflow boundary.

Finally, it is clear from Equation (50) that if $u_1 < a$ (the axial component of velocity is subsonic), then one of the characteristic lines defined by Equation (50b), namely that which corresponds to the upstream traveling wave surfaces, $dx_1/dt = u_1 - a$, originates downstream of the boundary, while the other, namely that corresponding to downstream traveling waves, $dx_1/dt = u_1 + a$, always originates upstream of the boundary, as depicted in Figure (3). On the other hand, if $u_1 > a$ (the axial component of velocity is supersonic), then both wave surfaces originate upstream of the boundary surface. Since the characteristics which originate outside the computational plane must be replaced by corresponding boundary conditions, closure of the inflow/outflow boundary condition statement depends on the axial component of the local Mach number. The required boundary conditions are summarized in Table 2. The normally anticipated situation for an arc tunnel or similar device consists of cases (1a), a subsonic inflow boundary at the plenum entrance, and (2b), a supersonic outflow boundary at the nozzle exit. However, the existing formulation includes all four (4) possibilities.

TABLE 2. BOUNDARY CONDITIONS AT THE INFLOW AND OUTFLOW STATIONS.

Boundary \ Local Mach Number	(a) Subsonic ($u_1 < a$)	(b) Supersonic ($u_1 > a$)
(1) Inflow (Plenum Entrance)	p T u_2 or (u_2/u_1) or $(\xi \text{ and } \eta)$ $u_3 \quad (j = 1)$ γ_i T_{v_i}	p T u_1 u_2 $u_3 (j=1)$ γ_i T_{v_i}
(2) Outflow (Nozzle Exit)	p	None

Equation (50a) is integrated along the characteristic lines (50b) which originate within the computational domain, e.g., along $dx_1/dt = u - a$ at the inflow boundary and along both $dx_1/dt = u_1 \pm a$ at the outflow station, to complete the solution at these boundary points. It is emphasized that this procedure avoids the need to evaluate derivatives at the boundary points by non-centered approximations, or to devise heuristic procedures such as extrapolation of interior point values to the boundary points. It does, however, assume constant entropy along streamlines over a zone adjacent to the boundaries of thickness less than a single grid spacing.

3. SOLID WALL BOUNDARY CONDITIONS

The boundary condition of impermeability is enforced at the walls, which requires the flow to be tangent to these surfaces. The reference-plane method-of-characteristics procedure can be applied along the walls by reorientation of the reference plane^(8b). However, for the present problem the alternate approach of using a modified version of the

interior point solution algorithm has been selected.^{8a} Enforcement of the boundary condition and determination of the flow solution along the walls is carried out in curvilinear surface-oriented coordinate system, in which (s,n) are coordinates parallel and normal to the surface, (v_s, v_n) are the corresponding velocity components, and ϕ is the surface angle measured with respect to the x_1 direction. The transformation between coordinate systems is given by:

$$\tan\phi = \frac{dr_w}{dx_1} \text{ at the wall} \quad (58)$$

$$u_1 = v_s \cos\phi - v_n \sin\phi \quad (59)$$

$$u_2 = v_s \sin\phi + v_n \cos\phi \quad (60)$$

$$\frac{\partial}{\partial x_1} = \cos\phi \frac{\partial}{\partial s} - \sin\phi \frac{\partial}{\partial n} \quad (61)$$

$$\frac{\partial}{\partial x_2} = \sin\phi \frac{\partial}{\partial s} + \cos\phi \frac{\partial}{\partial n} \quad (62)$$

The normal momentum equation is replaced by the condition $v_n = 0$. The members of the system of equations are solved by the interior point algorithm applied in the streamline coordinate system, as explained in Section 4.

4. AXIS BOUNDARY CONDITIONS

At the axis, the limit for $x_2 \rightarrow 0$, namely:

$$\frac{1}{x_2^j} \frac{\partial}{\partial x_2} (x_2^j f) = (j+1) \frac{\partial f}{\partial x_2} \quad (63)$$

is applied to the interior point equations of motion to derive the equations at the axis (or plane) of symmetry. The axis equations are then solved by the interior point algorithm, noting that at an axis (or plane) of symmetry.

$$\frac{\partial f}{\partial x_2} = 0, \quad f \neq u_2 \quad (64a)$$

$$\frac{\partial u_2}{\partial x_2} \neq 0 \quad (64b)$$

$$u_2 = 0 \quad (64c)$$

and therefore as $x_2 \rightarrow 0$:

$$f(-x_2) = f(x_2), \quad f \neq u_2 \quad (65a)$$

$$u_2(-x_2) = -u_2(x_2) \quad (65b)$$

SECTION 4

SOLUTION ALGORITHMS

1. INTERIOR POINTS AND STABILITY CRITERIA

The MacCormack scheme⁷ has been employed as the basic interior point solution method to solve the equation system (11), (12), (13), (14), (29) (or 37), (38) and (39). This method is now well known and widely used due to its combination of second-order accuracy and relative ease of coding, however, the basic elements are briefly reviewed herein.

The stated system of governing equations are written in the form:

$$\frac{\partial e}{\partial t} + \frac{\partial f}{\partial x_1} + \frac{\partial g}{\partial x_2} + h = 0 = \frac{\partial e}{\partial t} + A \frac{\partial f}{\partial \eta} + B \frac{\partial f}{\partial \xi} + C \frac{\partial g}{\partial \eta} + D \frac{\partial g}{\partial \xi} + h \quad (66)$$

where A,B,C and D are the components of the Jacobian of the transformation from (x_1, x_2) to (ξ, η) , and the arrays e,f,g and h are:

$$e = \rho [1, u_1, u_2, jx_2 u_3, T, \gamma_i, e_{v_1}] \quad (67)$$

$$f = [\rho u_1, (\rho u_1^2 + p), \rho u_1 u_2, j \rho u_1 u_3 x_2, \rho u_1 T, \rho u_1 \gamma_i, \rho u_1 e_{v_1}] \quad (68)$$

$$g = [\rho u_1 u_2, (\rho u_2^2 + p), j \rho u_2 u_3 x_2, \rho u_2 T, \rho u_2 \gamma_i, \rho u_2 e_{v_1}] \quad (69)$$

$$h = \rho [j u_2 / x_2, j u_1 u_2 / x_2, j (u_2^2 - u_3^2) / x_2, j u_2 u_3,$$

$$(T (\gamma_f - 1) \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} \right) + j \gamma_f T u_2 / x_2$$

$$+ (\sum \gamma_i \dot{e}_{vi} + \sum e_i \dot{\omega}_i / \rho) / C_v)$$

$$(ju_2 \gamma_i / x_2 - \dot{\omega}_i / \rho M W_i), (ju_2 e_{vi} / x_2 - \dot{e}_{vi})] \quad (70)$$

(In the equilibrium version of the program, the fifth component of the h array is redefined as

$$T(\gamma_e - 1) \left(\frac{\partial u_1}{\partial x} + \frac{\partial u_2}{\partial x} \right) + j \gamma_e T u_2 / x_2.$$

In addition, γ_i is redefined as $\tilde{\gamma}_i$, and the seventh component of the above stated system is dropped.)

A "predictor" value of $e(x_1, x_2, t + \Delta t)$ is obtained from a forward difference in time and non-centered differences in ξ and η . Using i, j subscript to denote an (ξ, η) grid point, and superscript n to denote time, t , and \tilde{e} to denote a "predictor" value, the first step of the two-step algorithm is:

$$\begin{aligned} \tilde{e}_{i,j}^{n+1} = & e_{i,j}^n + \Delta t \left\{ A(f_{i,j+1}^n - f_{i,j}^n) / \Delta \eta + B(f_{i+1,j}^n - f_{i,j}^n) / \Delta \xi \right. \\ & \left. + C(g_{i,j+1}^n - g_{i,j}^n) / \Delta \eta + D(g_{i+1,j}^n - g_{i,j}^n) / \Delta \xi + h_{i,j}^n \right\} \end{aligned} \quad (71)$$

The second step consists of essentially averaging the time derivatives evaluated at t and at $t+\Delta t$ giving a "corrector" value:

$$e_{i,j}^{n+1} = \frac{1}{2} \left\{ e_{i,j}^n + \tilde{e}_{i,j}^{n+1} + \Delta t \left[A(\tilde{f}_{k,j}^{n+1} - \tilde{f}_{i,j-1}^{n+1})/\Delta \eta \right. \right. \\ \left. \left. + B(\tilde{f}_{i,j}^{n+1} - \tilde{f}_{i-1,j}^{n+1})/\Delta \xi + C(\tilde{g}_{i,j}^{n+1} - \tilde{g}_{i,j-1}^{n+1})/\Delta \eta \right. \right. \\ \left. \left. + D(\tilde{g}_{i,j}^{n+1} - \tilde{g}_{i+1,j}^{n+1})/\Delta \xi + \tilde{h}_{i,j}^{n+1} \right] \right\} \quad (72)$$

This algorithm is stable when the well known CFL condition is met, without recourse to artificial damping or related filtering mechanisms. The CFL condition may be expanded in the context of the present system of equations to:

$$\Delta t = (\Delta t_{\text{wave}}^{-1} + \Delta t_{\text{chem}}^{-1} + \Delta t_{\text{vib}}^{-1})^{-1} \quad (73)$$

where

$$\Delta t_{\text{wave}} = \left[\frac{u_1}{\Delta x_1} + \frac{u_2}{\Delta x_2} + \frac{a}{\sqrt{\Delta x_1^2 + \Delta x_2^2}} \right]^{-1} \quad (74a)$$

$$\Delta t_{\text{chem}} = \left[(\dot{\omega}_i / \rho) \right]_{\text{max}}^{-1} \quad (74b)$$

$$\Delta t_{\text{vib}} = [\tau_i]_{\text{min}} \quad (74c)$$

The Landau-Teller rate constant τ_i is used for the vibrational time constant which neglects the possible effects of vibration-dissociation coupling. These are usually second-order type effects, except in extreme cases, such

as may be encountered during an initial transient in the solution. In this case, vibration-dissociation coupling should be neglected until the asymptotic portion of the unsteady solution is reached.

Note that there is no preferential order in which the spatial differences must be evaluated in the predictor and corrector steps. Therefore, a "rotating star" modification to the basic algorithm is sometimes employed.⁷ In this modification, the order in which points $(i+1,j)$, $(i-1,j)$, $(i,j-1)$ and $(i,j+1)$ are used is rotated, such that the sequence repeats every four (4) time steps. While it is true that this procedure avoids imparting any preferential bias to the solution associated with the order in which derivatives are evaluated, it is also the experience of the present investigators that it does not measurably reduce the eigenvalues of the stability matrix, and may, in fact, produce a slight cyclic behavior in the asymptotic solution, with a period of four time steps. This rotating star version of the algorithm is incorporated in the program as an option. Its utilization is left to the judgement of the user.

2. INLET PLANE

The inlet plane boundary conditions have two options for the user to choose. Either the static pressure distribution $P_{inlet}(x_2)$ or the total pressure distribution $p_{T_{inlet}}(x_2)$ may be specified. If the static pressure is given, it is accompanied by the static temperature distribution $T(x_2)$, but note that the pressure and temperature distributions should be consistent with requirements of the radial momentum equation. If the total pressure $P_T(x_2)$ is given then the total temperature field $T_T(x_2)$ must be specified. A distribution of axial velocity, $u_1(x_2)$ must also be specified, but it is only used if the inlet flow is supersonic (or becomes supersonic). In addition, the species concentration profile $\gamma_1(x_2)$ and the vibrational temperature profile $T_{v_1}(x_2)$ must also be given, as well as the normal and swirl velocity components, u_2 and u_3 , or the flow deflection angle u_2/u_1 (in lieu of u_2). Utilization of the total pressure option entails computation of the axial velocity $u_1(x_2,t)$ from the compatibility equation by iterating on the pressure field $p(x_2,t)$ at each time step. The density is obtained from:

$$\frac{p}{\rho \gamma} = \frac{P_T}{\rho_T \gamma} \quad (75)$$

where

$$\rho_T = (p_T / R_0 T_T) \overline{MW} \quad (76)$$

$$\gamma = \begin{cases} \gamma_f & \text{nonequilibrium} \\ \gamma_e & \text{equilibrium} \end{cases} \quad (77)$$

This option is therefore somewhat more time consuming, but presents an advantage where wall curvature at the inlet station makes it difficult to estimate the static pressure distribution which satisfies the radial momentum equation. On the other hand, the resulting static pressure and temperature distribution at the inlet may not be consistent with the specified species concentrations or vibrational temperatures.

3. EXIT PLANE SOLUTIONS

If the outlet is supersonic (as in the anticipated applications) no boundary condition should be imposed. The characteristic compatibility equations give all fluid mechanical components of the solution while the thermochemistry solution is obtained from a La Grangian type method (tracing outlet boundary point streamlines back into the computational domain at each time step).

For a subsonic exit condition, the exit pressure field must be prescribed, while the rest of the solution follows as above.

4. WALL POINTS

As mentioned earlier, the wall point boundary condition is satisfied by writing the equations in a streamline coordinate system along the wall. The normal momentum equation is replaced by the condition $v_n = 0$. The normal derivatives in the continuity, streamwise momentum and energy equations involve only the gradient of the normal component of velocity. These terms are approximated by a centered difference evaluated one-half grid spacing off the wall. Second order accuracy should be thereby retained, except in regions of very small radius of curvature (i.e., near points of discontinuous curvature).

Since the angular momentum, species conservation and vibrational energy equations become exact integrals along a wall, i.e., see Equations (55), they are solved in Lagrangian form:

$$rv_{\theta} = \text{constant} = [rv_{\theta}]_{(s-v_s\Delta t), (t-\Delta t)} \quad (78)$$

$$\gamma_i = \text{constant} + \int_{\Delta t} \dot{\gamma}_i / \rho \, dt \approx [\gamma_i + \dot{\gamma}_i \Delta t / \rho]_{(s-v_s\Delta t), (t-\Delta t)} \quad (79)$$

$$e_{v_i} = \text{constant} + \int_{\Delta t} \dot{e}_{v_i} \, dt \approx [e_{v_i} + \dot{e}_{v_i} \Delta t]_{(s-v_s\Delta t), (t-\Delta t)} \quad (80)$$

The bracketed quantities are evaluated at position $v_s\Delta t$ upstream of the wall grid point in question by linear interpolation of the known solution at time $t-\Delta t$.

SECTION 5

CAPABILITIES AND LIMITATIONS

Program R2D2 is designed to solve internal, inviscid, chemically reacting and vibrationally relaxing flows through two-dimensional (planar or axisymmetric) converging-diverging ducts. The thermochemistry components of the program have been derived from well established theory and utilize subroutines from an existing one-dimensional steady flow program¹²⁻¹⁴. Thus, the thermochemical aspects of the solution should possess a degree of accuracy consistent with the limitations of the chemical kinetic data and thermodynamic properties and with the accuracy of the fluid-mechanical properties of the solution.

In regard to the accuracy of the fluid mechanical properties of the solution, it should be pointed out that few, if any, "benchmark" type solutions are available for two-dimensional, subsonic, swirling, internal flows. Numerical solutions are seldom stated with sufficient information on boundary conditions and rate of convergence with respect to grid size to permit comparisons to be made. Experimental data, on the other hand, almost invariably include viscous effects which are not incorporated in the analytical model. However, virtually exact inviscid solution techniques are available¹⁷ for the interesting, and difficult, case of transonic flows near the throat of nozzles having circular arc wall contours, based on series expansions about sonic flow. Comparisons have been carried out using a perfect gas (i.e., frozen flow) version of the present program for the case of an axisymmetric duct having a circular arc wall contour of radius $R=10r^*$, where R is the radius of curvature of the wall and r^* is the radius of the throat.

The computational domain was defined to extend over the axial range $-0.19 \leq z/r^* \leq 0.19$. The boundary conditions imposed at the inlet station consisted of uniform total Pressure, uniform total temperature, zero vorticity and zero swirl. A uniform back pressure corresponding to a Mach number of 1.02 was specified at the exit station to ensure that the solution converged on the supersonic branch in the diverging section (although in fact this turned out to be unnecessary since the solution never jumped to the subsonic branch).

A grid network having 5 columns ($\Delta z = .0475r^*$) and 20 rows ($\Delta r = .05263r^*$ at the throat) was selected initially. The solution became asymptotic after 400 time

steps (i.e., the solution after 500 steps was virtually indistinguishable from that at 400 steps). The Mach number distributions along the axis and duct wall are compared with the solution techniques from Reference (17) in Figure (4). Note that in this case the latter technique produces very nearly linear variations and is, therefore, highly accurate (i.e., the nonlinear terms included in the expansion are small but not negligible).

The differences between the present solution and the analytical solution can be put in a proper frame of reference by noting that the maximum error in mass flow rate, which occurs at the station $z=.095r^*$, is 4/100 of 1% and that the average error for the 5 grid lines is 1/100 of 1%. Nevertheless, the fact that the maximum differences occurred at the grid lines adjacent to the inlet and outlet stations motivated a second computation with 9 grid columns and 20 rows, which required 800 time steps to become asymptotic. As can also be seen in Figure (4), the second solution was brought into substantially improved agreement with the analytical solution. The maximum and average errors in mass flow rate were both halved. The radial distribution of Mach number is shown in Figure (5) at station $z=.095r^*$; the agreement obtained in the second calculation is virtually perfect.

Thus a high degree of confidence can be placed in the fluid mechanical aspects of the present technique if an adequate grid spacing is employed. However, the judgement as to adequacy of the grid spacing must be based on some integral properties of the solution, such as conservation of mass. It appears that errors on the order of .04% in mass flow rate from station-to-station may signal departure from an "exact" solution. The magnitude of the error which is tolerable in any particular case must be determined in the context of the problem.

The running time required to execute cases with a large number of chemical species may be a significant deterrent to the routine use of Program R2D2. The program is presently set up to run a system representing air, with three elements (oxygen, nitrogen and argon), 8 chemical species, 10 chemical reactions, and three vibrationally excited molecules. The execution time on a CDC 6600 mainframe is on the order of 0.15 seconds per grid point per time step, as compared to about 0.002 seconds for a perfect gas. The amount of time spent is therefore disproportionately greater than the increase in number of equations. The calculation of rate constants, species production terms and vibrational relaxation terms is believed to be the primary contributor to the difference. Since these calculations

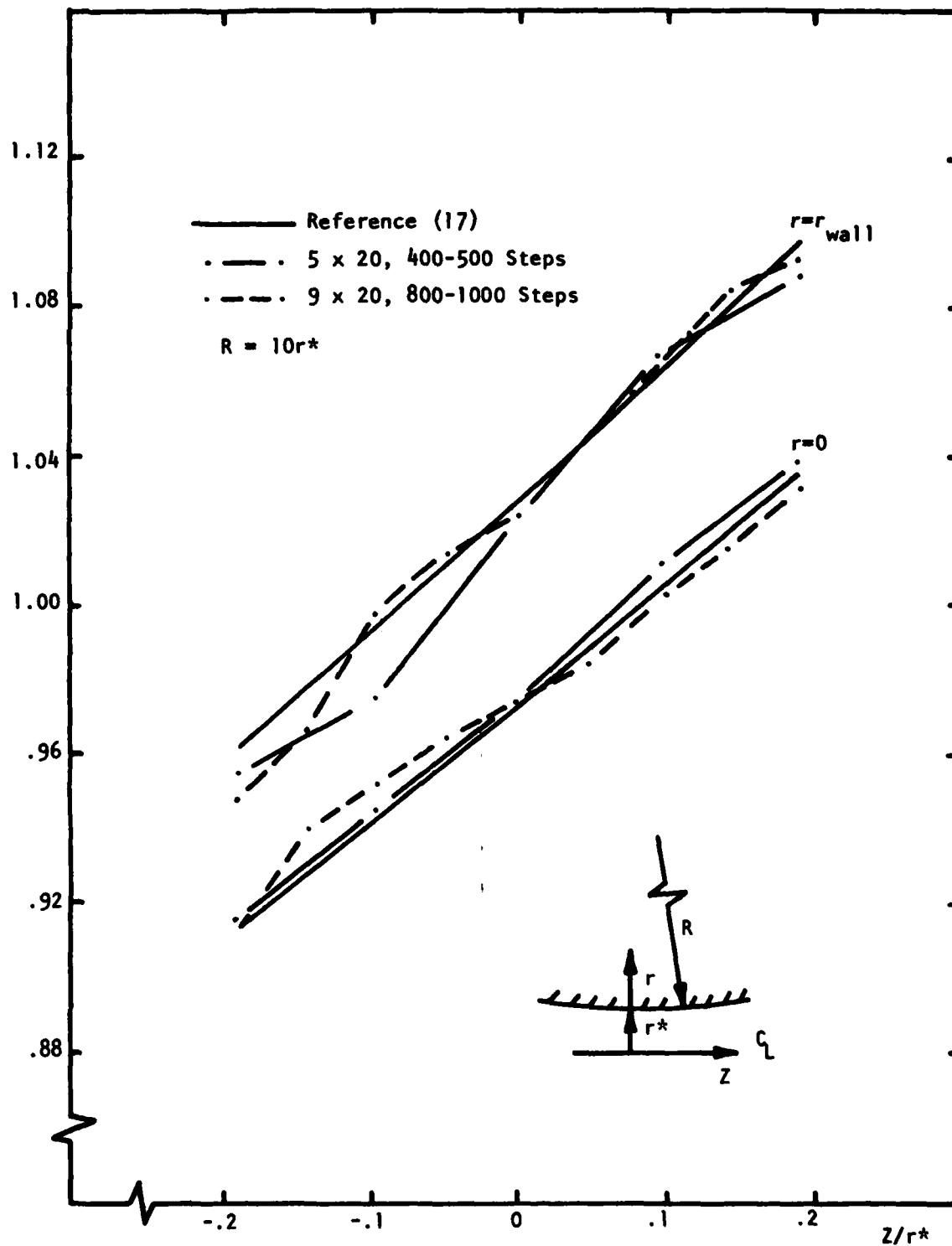


FIGURE 4. AXIAL DISTRIBUTION OF MACH NUMBER ALONG WALL AND AXIS OF CIRCULAR ARC CONVERGING-DIVERGING DUCT

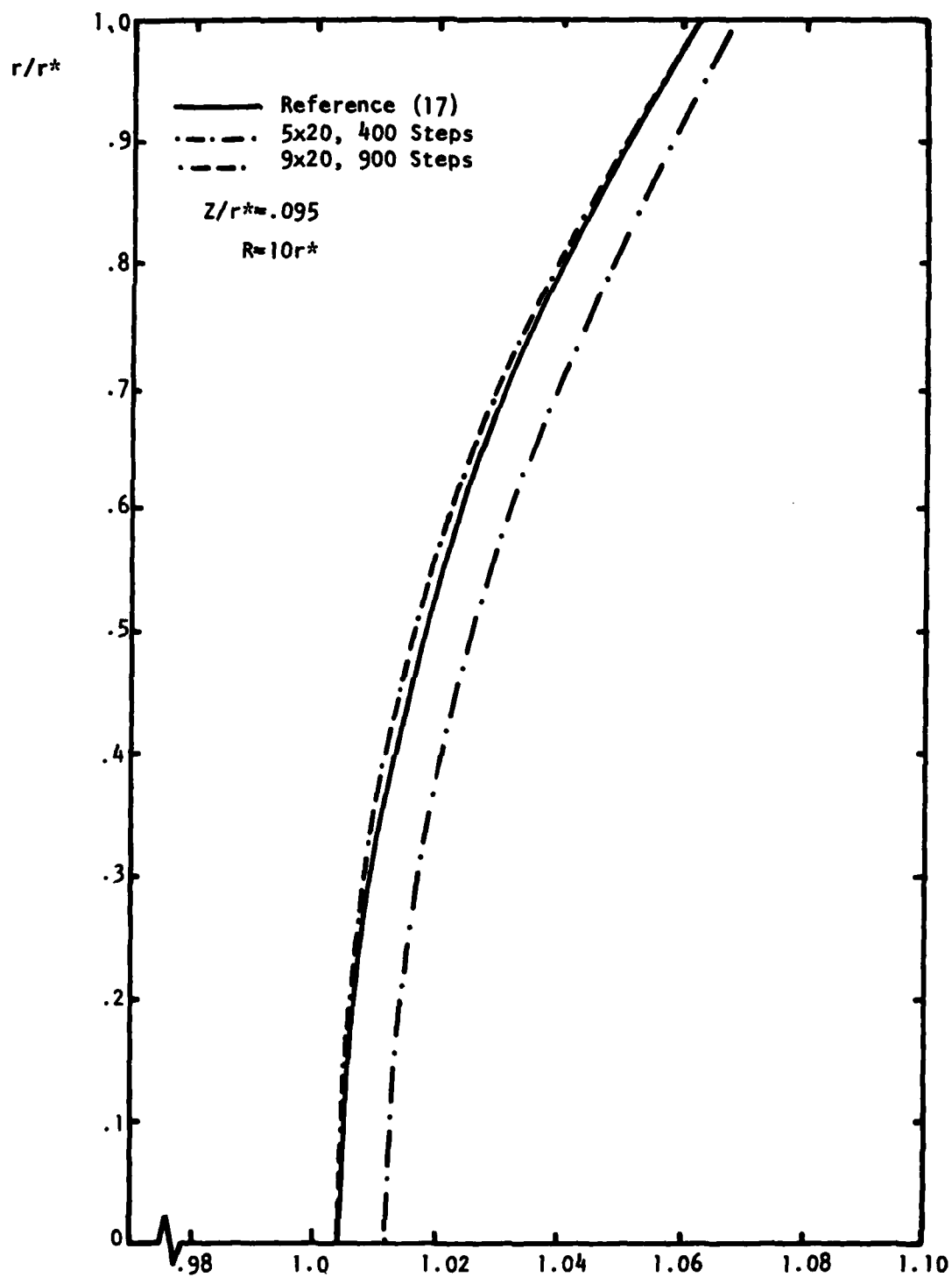


FIGURE 5. RADIAL DISTRIBUTION OF MACH NUMBER AT $Z/r^* = .095$ IN A CIRCULAR ARC CONVERGING-DIVERGING DUCT.

cannot be reduced substantially while retaining the desired generality in the thermochemical model, the only savings can be in reducing the number of grid points and number of time steps. The former is dictated by accuracy requirements and the latter by the CFL stability requirement, which couples it, in turn, to the number of grid points.

It is pointed out that the time to reach an asymptotic steady state is associated with the time for waves of both families to travel between the inlet and outlet. Thus a subsonic solution is generally the slowest to converge while a supersonic solution (for which both families of waves travel downstream) is faster, with the required time decreasing inversely with Mach number. Thus, the time for a solution to a mixed flow problem, such as a converging-diverging duct, to reach an asymptotic state is controlled by the subsonic part of the solution. This suggests that cases involving a short plenum and a long, hypersonic nozzle, for example, can be most efficiently executed by treating only the plenum, throat and a portion of the nozzle sufficiently long to ensure a supersonic flow at the exit plane. The exit plane solution obtained in the asymptotic limit for this case can then be used as inlet station conditions for the next segment of the nozzle, which will then converge to its asymptote more quickly than if it had been treated as part of the first case. Alternatively, a more efficient technique, such as the method-of-characteristics, can also be used for the hypersonic expansion.

The program can accommodate arbitrary thermochemical systems by replacing the chemical kinetic and thermodynamic data packages, which is discussed in greater detail in the second volume of this report. However, it is specifically designed to accommodate a variety of data packages representing frequently used thermochemical systems.

SECTION 6

CONCLUSIONS AND RECOMMENDATIONS

A program for solution of two-dimensional (planar or axisymmetric) internal flows of inviscid, chemically reacting and/or vibrationally relaxing mixtures of gases has been developed. The program has been specifically formulated for application to arc-driven wind tunnels; it therefore includes consideration of swirl as well as axial and radial velocity components, and of nonuniform, subsonic plenum conditions. The chemical system presently incorporates an 8 species model of air, with 10 chemical reactions and 3 vibrationally relaxing molecules. However, the program has been structured to readily admit other chemical systems by redefinition of the thermodynamic and chemical kinetic data. In addition, arbitrary planar or axisymmetric ducts, including discontinuous wall slopes, can be considered. A simple nonorthogonal grid is employed in the finite-difference solution algorithm, but other grid generation schemes are readily admissible, so long as they map the duct boundaries to boundaries of the computational domain and define the components of the Jacobian of the transformation at every grid point.

The conservation laws for unsteady flows are solved subject to steady boundary conditions, with the objective of determining the asymptotic steady state. Proper formulation of the inlet and exit station boundary conditions is discussed for both subsonic and supersonic flows. The program can treat arbitrary combinations of conditions. Uniqueness can only be guaranteed for a choked subsonic or a supersonic flow, however this encompasses the intended application of the program. In an unchoked subsonic flow the program will presumably converge on the solution closest to the initial conditions, whereas in all other cases it should be independent of the initial conditions. Provisions to restart the solution with the same or different boundary conditions have been made, with a view toward minimizing the computer time requirement. An explicit finite difference algorithm has been used, which therefore places a severe restriction on the permissible time step. Consequently, a large number of time steps

may be required to reach an asymptotic solution, which can require very substantial amounts of computer time. The time requirement depends, of course, on the grid size, the chemical system, the boundary conditions and the initial conditions. However, execution times on the order of .15 seconds per grid point per time step have been encountered, with the considered air model on a CDC 6600 mainframe computer system. Since the total number of grid points may be of order 10^2 and the total number of time steps of order 10^3 , the total running time on this computer can be of the order of four hours.

In view of the substantial running time the present version of the program requires, adoption of an implicit solution algorithm is recommended. Removal of the CFL stability restriction associated with the explicit method presently used could probably permit an order of magnitude reduction in the number of time steps needed to reach an asymptotic state. On the other hand, implicit techniques couple the system of equations, and in a chemically reacting, vibrationally relaxing flow the matrix operations may partially offset the reduction in number of time steps.

The present flow model is also clearly idealized with respect to its intended application in the sense that it neglects such important phenomena as turbulence, liquid phase material from the melting arc, particulate matter in the air stream, ionization nonequilibrium, etc., as well as azimuthal nonuniformities in the flow. These phenomena could also be incorporated in the program, although at the expense of additional computer resources, in varying degrees. However, the need to make the present version of the program a more practical tool for routine use appears to be the first priority. Nevertheless, it should be clearly recognized that this program possesses a two-dimensional capability which one-dimensional analyses cannot provide (especially with regard to swirl effects and abrupt cross-sectional area variations), but which inevitably requires more substantial computer resources than a one-dimensional analysis.

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